Isoflupredone, bis-MO-tris-TMS

Inchi: InChI=1S/C32H57FN2O5Si3/c1-29-18-16-24(34-36-3)20-23(29)14-15-26-25-17-19-31(40
InchiKey: YIWPTVOOWPWARJ-XZVCHNANSA-N
Formula: C32H57FN2O5Si3
SMILES: CON=C1C=CC2(C)C(=C1)CCC1C3CCC(O[Si](C)(C)C)(C(CO[Si](C)(C)C)=NOC)C3(C)C
Mol. weight [g/mol]: 653.06

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.62		Crippen Method
logp	8.094		Crippen Method
rinpol	3000.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R558055&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices